

USE A SUPERVISED MACHINE LEARNING APPROACH TO INFER A MAPPING FUNCTION F THAT TRANSFORMS THE INPUT FEATURES VECTOR FOR EACH PRODUCT OF THE TRAINING SUBSET OF PRODUCTS TO THE CORRESPONDING AT LEAST ONE PROPERTY FOR EACH PRODUCT OF THE TRAINING SUBSET OF PRODUCTS

U160

IDENTIFY BUILDING BLOCK SETS FOR A PLURALITY OF ADDITIONAL PRODUCTS OF THE COMBINATORIAL LIBRARY

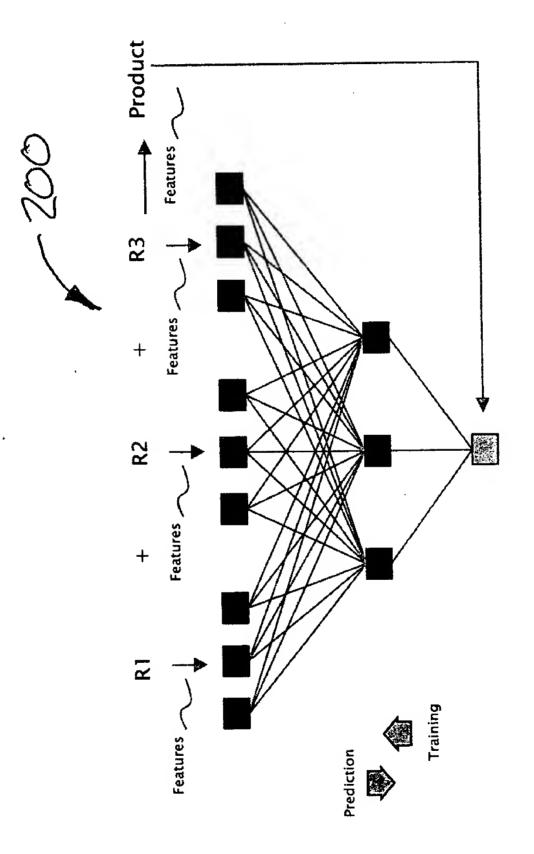
170

FORM INPUT FEATURES VECTORS FOR THE PLURALITY OF ADDITIONAL PRODUCTS FROM THE BUILDING BLOCK SETS FOR THE PLURALITY OF ADDITIONAL PRODUCTS

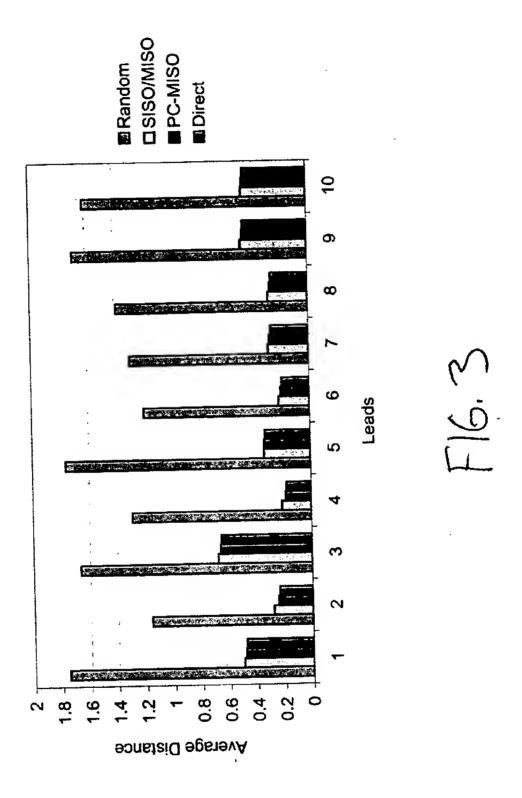
180

TRANSFORM THE INPUT FEATURES VECTORS FOR THE PLURALITY OF ADDITIONAL PRODUCTS USING THE MAPPING FUNCTION F TO OBTAIN AT LEAST ONE ESTIMATE PROPERTY FOR EACH OF THE PLURALITY OF ADDITIONAL PRODUCTS

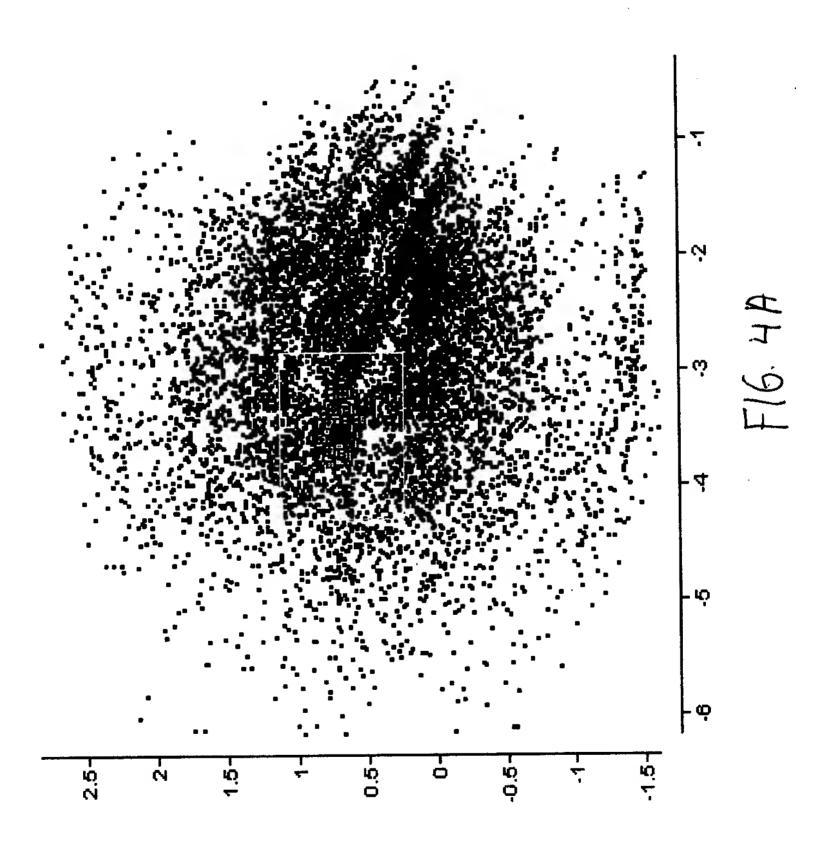
1-190.



F16.2



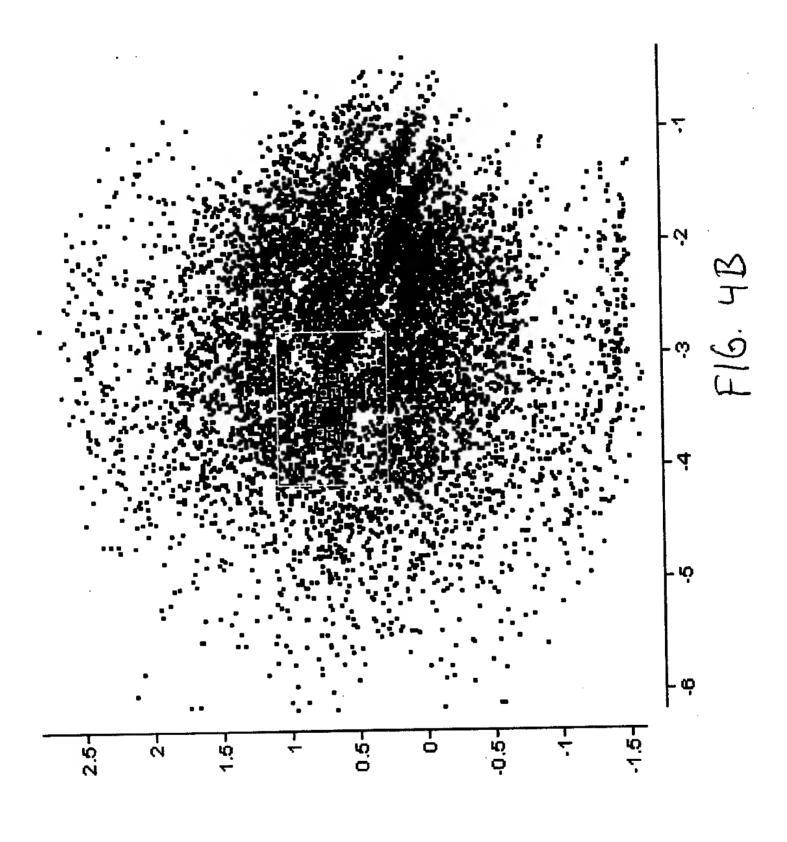
.)

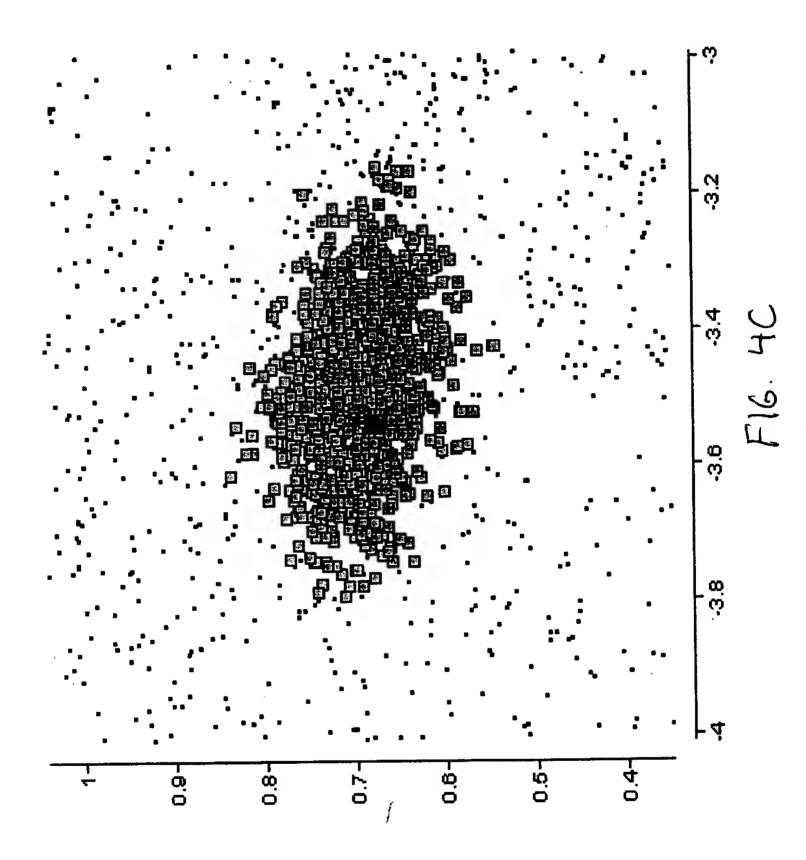


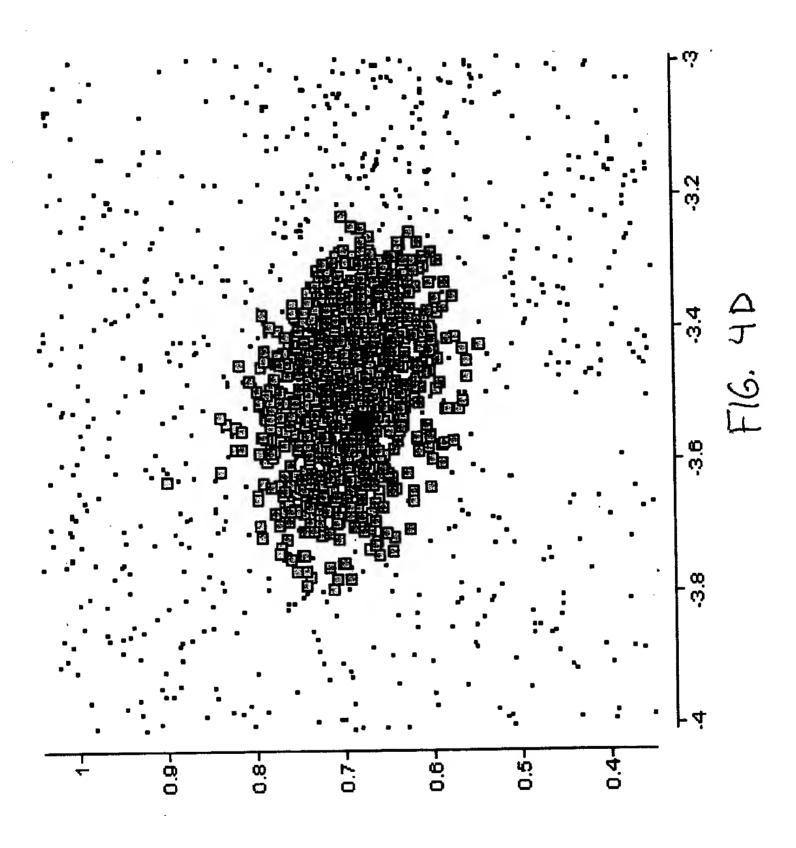
•

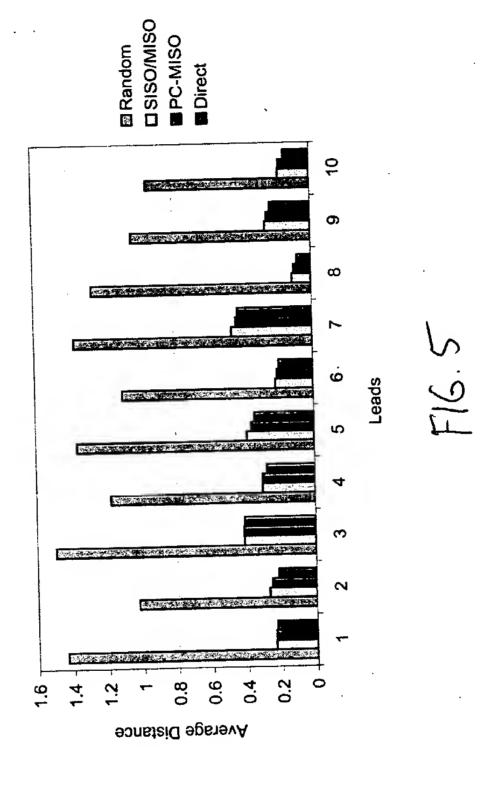
•

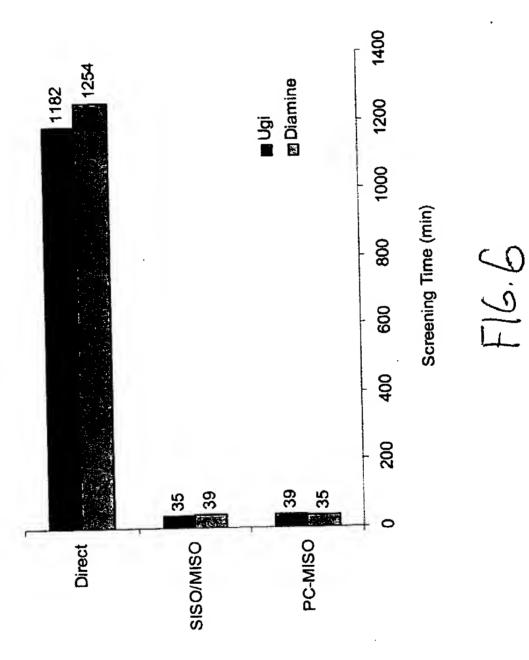
.

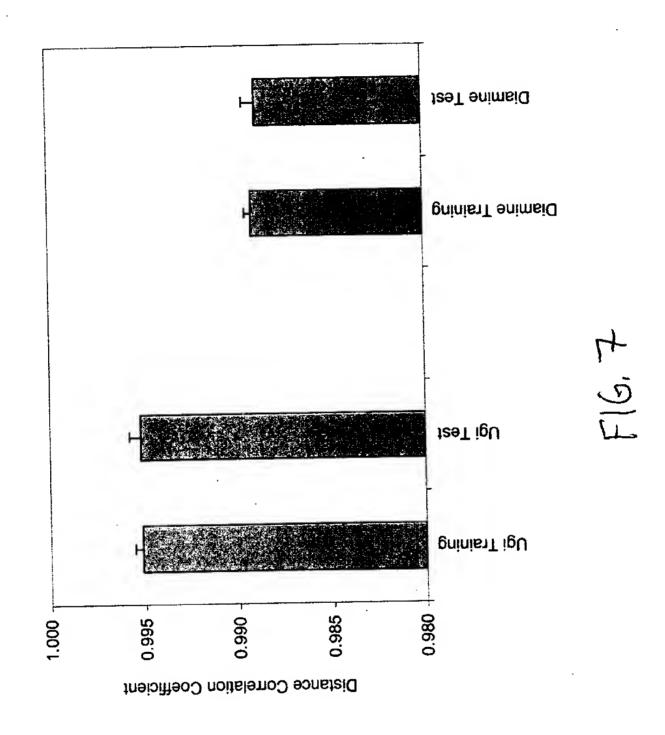


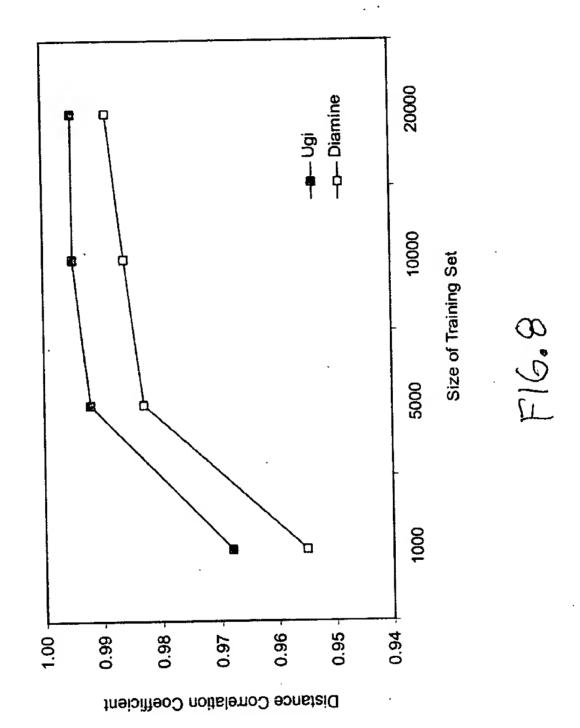












No. atoms
No. elements
Molecular weight
Chi path 1
Chi path 2
Chi path 3
Chi path 4
Chi path 5
Chi path 6
Chi path 7
Chi path 8
Chi path 9
Chi path 10
Chi cluster 3
Chi path/cluster 4
Val chi 0
Val chi path 1
Val chi path 2
Val chi path 3
Val chi path 4
Val chi path 5
Val chi path 6

F16. 9A

f+:

: :;

		Coro	Coro	Core	Contract
		Octo	Octo	OCTAL	OCTAI
		Training	Test	Training	Test
Index	Descriptor	R-	R.	R.	R*
26	Val chi path 7	0.773	0.775	0.961	0.905
27	Val chi path 8	0.619	0.621	0.890	0.889
28	Val chi path 9	0.349	0.328	0.910	0.910
29	Val chi path 10	0.222	0.201	0.921	0.920
30	Val chi cluster 3	0.994	0.994		
31	Val chi cluster 4	0.993	0.993		
32	Val chi path/cluster 4	886.0	0.989	·	
33	Chi chain 3	1.000	1.000		
34	Chi chain 4	1.000	1.000		
35	Chi chain 5	0.979	0.978		
36	Chi chain 6	0.995	0.995		
37	Chi chain 7	0.999	0.999		
38	Chi chain 8	1.000	1.000		
39	Chi chain 9	0.999	666.0		
40	Chi chain 10	0.999	0.998		
.4 <u>1</u>	val chi chain 3	1.000	1.000		
42	val chi chain 4	1.000	1.000		
43	val chi chain 5	0.994	966.0		
44	val chi chain 6	0.994	0.995		
45	val chi chain 7	0.998	0.998		
46	val chi chain 8	1.000	1.000		
47	val chi chain 9	0.997	0.998		
4.8	val chi chain 10	0.986	0.980		
49	subgraph count path 2	966'0	0.997		
50	subgraph count path 3	066.0	0.660	*	

F16. 9B

124

Index   Descriptor   Rg <sup>2</sup> Rg <sup>2</sup> Rg <sup>2</sup> Training Rg <sup>2</sup> Rg <sup>2</sup> Test Rg <sup>2</sup> Rg <sup>2</sup> Training Rg <sup>2</sup> Rg <sup>2</sup> Test Rg <sup>2</sup> Rg			SISO	SISO	MISO .	MISO
Subgraph count path 4   0.957   0.960     subgraph count path 5   0.914   0.918     subgraph count path 6   0.837   0.844   0.909     subgraph count path 8   0.582   0.770   0.892     subgraph count path 8   0.582   0.599   0.907     subgraph count path 9   0.446   0.448   0.933     subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.947     subgraph count cluster 4   0.991   0.991   0.991     subgraph count ring 3   1.000   1.000   1.000     subgraph count ring 6   0.994   0.995   0.995     subgraph count ring 6   0.994   0.995   0.995     subgraph count ring 8   1.000   1.000   1.000     subgraph count ring 9   1.000   1.000   1.000     subgraph count ring 10   0.995   0.995   0.995     kappa 1   0.097   0.990   0.990     kappa 2   0.907	,	4	Training	Test	Training 5.2	Test
subgraph count path 4   0.957   0.960     subgraph count path 5   0.914   0.918     subgraph count path 6   0.837   0.844   0.909     subgraph count path 8   0.582   0.599   0.907     subgraph count path 9   0.446   0.448   0.933     subgraph count path 10   0.366   0.383   0.947     subgraph count path 10   0.366   0.383   0.947     subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.997     subgraph count ring 3   1.000   1.000   0.995     subgraph count ring 4   0.995   0.995   0.995     subgraph count ring 6   0.994   0.995   0.995     subgraph count ring 8   1.000   1.000   1.000     subgraph count ring 9   1.000   1.000   1.000     subgraph count ring 10   0.999   0.995   0.995     kappa 2   0.907   0.990   0.990     kappa alpha 1   0.987	Index	Descriptor	꾹	찪	K	ᅺ
subgraph count path 5   0.914   0.918     subgraph count path 6   0.837   0.844   0.909     subgraph count path 7   0.752   0.770   0.892     subgraph count path 8   0.582   0.599   0.907     subgraph count path 10   0.366   0.383   0.947     subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.947     subgraph count path/cluster 4   0.980   0.990   0.995     subgraph count ring 3   1.000   1.000   1.000     subgraph count ring 4   1.000   1.000   1.000     subgraph count ring 5   0.995   0.995   0.995     subgraph count ring 8   1.000   1.000   1.000     subgraph count ring 9   1.000   1.000   1.000     subgraph count ring 10   0.999   0.999   0.999     kappa 2   0.090   0.990   0.990     kappa 3   0.709   0.709   0.709     kappa alpha 1   <	51	subgraph count path 4	0.957	0.960		
subgraph count path 6   0.837   0.844   0.909     subgraph count path 7   0.752   0.770   0.892     subgraph count path 8   0.582   0.599   0.907     subgraph count path 9   0.446   0.448   0.933     subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.947     subgraph count path/cluster 4   0.991   0.990   0.947     subgraph count ring 3   1.000   1.000   1.000     subgraph count ring 4   1.000   1.000   1.000     subgraph count ring 5   0.995   0.995   0.995     subgraph count ring 6   0.994   0.995   0.995     subgraph count ring 10   0.999   0.999   0.999     kappa 0   0.090   0.999   0.999     kappa 1   0.999   0.999   0.998     kappa 2   0.997   0.998   0.998     kappa alpha 1   0.987   0.987   0.990     kappa alpha 2   <	52	subgraph count path 5	0.914	0.918		
subgraph count path 7   0.752   0.770   0.892     subgraph count path 8   0.582   0.599   0.907     subgraph count path 10   0.446   0.448   0.933     subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.947     subgraph count cluster 4   0.991   0.991   0.991     subgraph count ring 3   1.000   1.000   1.000     subgraph count ring 4   1.000   1.000   1.000     subgraph count ring 5   0.995   0.995   subgraph count ring 6   0.994   0.995     subgraph count ring 8   1.000   1.000   1.000     subgraph count ring 9   1.000   1.000   1.000     subgraph count ring 10   0.999   0.999   0.999     kappa 1   0.991   0.990   0.990     kappa 2   0.991   0.991   0.907     kappa 3   0.709   0.710   0.774     kappa alpha 1   0.685   0.897   0.774	53	subgraph count path 6	0.837	0.844	0.909	0.905
subgraph count path 8   0.582   0.599   0.907     subgraph count path 9   0.446   0.448   0.933     subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.947     subgraph count cluster 4   0.991   0.991   0.991     subgraph count ring 3   1.000   1.000   1.000     subgraph count ring 4   1.000   1.000   1.000     subgraph count ring 5   0.995   0.995   0.995     subgraph count ring 6   0.994   0.995   0.995     subgraph count ring 8   1.000   1.000   1.000     subgraph count ring 9   1.000   1.000   0.995     kappa 0   0.999   0.999   0.999     kappa 1   0.991   0.992   0.996     kappa 2   0.997   0.992   0.996     kappa 3   0.709   0.710   0.806     kappa alpha 1   0.987   0.897   0.774     kappa alpha 3   0.685	54	subgraph count path 7	0.752	0.770	0.892	0.887
subgraph count path 9   0.446   0.448   0.933     subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.947     subgraph count cluster 4   0.991   0.991   0.991     subgraph count ring 3   1.000   1.000   1.000     subgraph count ring 4   1.000   1.000   1.000     subgraph count ring 5   0.995   0.995   0.995     subgraph count ring 6   0.994   0.995   0.995     subgraph count ring 8   1.000   1.000   1.000     subgraph count ring 9   1.000   1.000   0.999     kappa 0   0.999   0.999   0.999     kappa 1   0.990   0.990   0.990     kappa 2   0.900   0.900   0.908     kappa 3   0.709   0.710   0.806     kappa alpha 1   0.987   0.987   0.960     kappa alpha 3   0.685   0.686   0.774	55	subgraph count path 8	0.582	0.599	0.907	0.906
subgraph count path 10   0.366   0.383   0.947     subgraph count cluster 3   0.994   0.995   0.997     subgraph count cluster 4   0.991   0.991   0.995     subgraph count ring 3   1.000   1.000   1.000     subgraph count ring 5   0.995   0.995   0.995     subgraph count ring 6   0.994   0.995   0.995     subgraph count ring 7   1.000   1.000   1.000     subgraph count ring 8   1.000   1.000   1.000     subgraph count ring 9   1.000   1.000   0.995     kappa 0   0.980   0.999   0.999     kappa 1   0.991   0.992   0.908     kappa 2   0.907   0.908   0.906     kappa 2   0.907   0.908   0.908     kappa 3   0.709   0.710   0.806     kappa alpha 1   0.987   0.987   0.960     kappa alpha 2   0.685   0.774   0.774	56	subgraph count path 9	0.446	0.448	0.933	0.932
subgraph count cluster 3   0.994   0.995     subgraph count cluster 4   0.991   0.991     subgraph count path/cluster 4   0.980   0.980     subgraph count ring 3   1.000   1.000     subgraph count ring 5   0.995   0.995     subgraph count ring 6   0.994   0.995     subgraph count ring 8   1.000   1.000     subgraph count ring 9   1.000   1.000     subgraph count ring 10   0.999   0.999     kappa 1   0.980   0.999     kappa 2   0.991   0.998     kappa 3   0.709   0.710   0.80%     kappa 3   0.709   0.710   0.960     kappa alpha 1   0.887   0.897   0.744	57	subgraph count path 10	0.366	0.383	0.947	0.945
subgraph count cluster 4   0.991   0.991     subgraph count ring 3   1.000   1.000     . subgraph count ring 4   1.000   1.000     subgraph count ring 5   0.995   0.995     subgraph count ring 6   0.994   0.995     subgraph count ring 7   1.000   1.000     subgraph count ring 8   1.000   1.000     subgraph count ring 9   1.000   1.000     subgraph count ring 9   1.000   0.980     kappa 0   0.980   0.980     kappa 1   0.980   0.980     kappa 2   0.907   0.908     kappa 3   0.709   0.710     kappa alpha 1   0.987   0.960     kappa alpha 2   0.895   0.897     kappa alpha 3   0.685   0.774	58	subgraph count cluster 3	0.994	0.995		
subgraph count path/cluster 4   0.980   0.980     subgraph count ring 3   1.000   1.000     subgraph count ring 4   1.000   1.000     subgraph count ring 5   0.995   0.995     subgraph count ring 6   0.994   0.995     subgraph count ring 8   1.000   1.000     subgraph count ring 9   1.000   1.000     subgraph count ring 10   0.999   0.999     kappa 1   0.980   0.980     kappa 2   0.991   0.908     kappa 2   0.907   0.908     kappa 3   0.709   0.710     kappa alpha 1   0.987   0.987     kappa alpha 2   0.895   0.897     kappa alpha 3   0.685   0.774	59	subgraph count cluster 4	0.991	0.991		
subgraph count ring 3 1.000 1.000   subgraph count ring 5 0.995 0.995   subgraph count ring 6 0.994 0.995   subgraph count ring 7 1.000 1.000   subgraph count ring 8 1.000 1.000   subgraph count ring 9 1.000 1.000   subgraph count ring 10 0.999 0.999   kappa 0 0.980 0.980   kappa 1 0.991 0.992   kappa 2 0.907 0.908   kappa 3 0.709 0.709   kappa alpha 1 0.987 0.987   kappa alpha 2 0.895 0.897   kappa alpha 3 0.685 0.774	09	subgraph count path/cluster 4	0.980	0.980		
subgraph count ring 4 1.000 1.000   subgraph count ring 5 0.995 0.995   subgraph count ring 7 1.000 1.000   subgraph count ring 8 1.000 1.000   subgraph count ring 9 1.000 1.000   kappa 0 0.999 0.999   kappa 1 0.980 0.909   kappa 2 0.907 0.908   kappa 3 0.709 0.710   kappa 3 0.709 0.710   kappa 3 0.709 0.710   kappa alpha 1 0.987 0.960   kappa alpha 2 0.685 0.686   kappa alpha 3 0.685 0.686	61.	subgraph count ring 3	1.000	1.000		
subgraph count ring 5   0.995   0.995     subgraph count ring 6   0.994   0.995     subgraph count ring 7   1.000   1.000     subgraph count ring 9   1.000   1.000     subgraph count ring 10   0.999   0.999     kappa 0   0.980   0.980     kappa 1   0.991   0.908     kappa 2   0.907   0.908     kappa 3   0.709   0.710   0.806     kappa alpha 1   0.987   0.987   0.960     kappa alpha 2   0.895   0.897   0.774     kappa alpha 3   0.685   0.686   0.774	62		1.000	1.000		
subgraph count ring 6 0.994 0.995   subgraph count ring 7 1.000 1.000   subgraph count ring 8 1.000 1.000   subgraph count ring 10 0.999 0.999   subgraph count ring 10 0.980 0.980   kappa 1 0.991 0.902   kappa 2 0.907 0.908   kappa 3 0.709 0.710   kappa 3 0.709 0.987   kappa alpha 1 0.987 0.987   kappa alpha 2 0.895 0.897   kappa alpha 3 0.685 0.774	63.	subgraph count ring 5	0.995	0.995		
subgraph count ring 7 1.000 1.000   subgraph count ring 8 1.000 1.000   subgraph count ring 10 0.999 0.999   kappa 0 0.980 0.980   kappa 1 0.991 0.902   kappa 2 0.907 0.908   kappa 3 0.709 0.710 0.806   kappa alpha 1 0.987 0.987 0.960   kappa alpha 2 0.895 0.897 0.960   kappa alpha 3 0.685 0.686 0.774	64	subgraph count ring 6	0.994	0.995		
subgraph count ring 8 1.000 1.000   subgraph count ring 10 0.999 0.999   kappa 0 0.980 0.980   kappa 1 0.991 0.992   kappa 2 0.907 0.908   kappa 3 0.709 0.709   kappa alpha 1 0.987 0.987   kappa alpha 2 0.895 0.897   kappa alpha 3 0.685 0.686   kappa alpha 3 0.685 0.686	65	subgraph count ring 7	1.000	1.000		
subgraph count ring 9 1.000 1.000   subgraph count ring 10 0.999 0.999   kappa 0 0.980 0.980   kappa 1 0.991 0.902   kappa 2 0.907 0.908   kappa 3 0.709 0.710 0.806   kappa alpha 1 0.987 0.987 0.960   kappa alpha 2 0.685 0.686 0.774	.99	subgraph count ring 8	1.000	1.000		
subgraph count ring 10 0.999 0.999 0.999   kappa 0 0.980 0.980 0.980   kappa 1 0.991 0.992 0.908   kappa 2 0.907 0.908 0.806   kappa 3 0.709 0.710 0.806   kappa alpha 1 0.987 0.980   kappa alpha 2 0.895 0.897 0.960   kappa alpha 3 0.685 0.686 0.774	:29	subgraph count ring 9	1.000	1,000		•
kappa 0 0.980 0.980 0.980   kappa 1 0.991 0.992 —   kappa 2 0.907 0.908 —   kappa 3 0.709 0.710 0.806   kappa alpha 1 0.987 0.987 0.960   kappa alpha 2 0.895 0.897 0.960   kappa alpha 3 0.685 0.686 0.774	89		0.999	0.999		
kappa 1 0.991 0.992   kappa 2 0.907 0.908   kappa 3 0.709 0.710 0.806   kappa alpha 1 0.987 0.987 0.960   kappa alpha 2 0.895 0.897 0.960   kappa alpha 3 0.685 0.686 0.774	69		0.980	0.980	·	
kappa 2 0.907 0.908   'kappa 3 0.709 0.710 0.806   kappa alpha 1 0.987 0.987 0.960   kappa alpha 2 0.895 0.897 0.960   kappa alpha 3 0.685 0.686 0.774	7.3	kappa I	0.991	0.992		
'kappa 3 0.709 0.710 0.806   kappa alpha 2 0.987 0.987   kappa alpha 3 0.685 0.686 0.774	71	kappa 2	0.907	0.908		•
kappa alpha 1 0.987 0.987   kappa alpha 3 0.895 0.897 0.960   kappa alpha 3 0.685 0.686 0.774	72	kappa 3	0.709	0.710	0.80€	0.799
kappa alpha 2 0.895 0.897 0.960 kappa alpha 3 0.685 0.686 0.774	73	kappa alpha 1	0.987	0.987	,	
kappa alpha 3 0.685 0.686 0.774	74	kappa alpha 2	0.895	0.897	0.960	0.955
	75%	kappa alpha 3	0.685	989.0	0.774	0.770

F16. 9C

			SISO	SISO	MISO	MISO
<u> </u>	<u>:</u> `		Training	Test	Training	Test
	Index	Descriptor	$\mathbb{R}^2$	R <sup>2</sup>	R <sup>2</sup>	χ <sub>2</sub>
L	76	Wiener path no.	0.967	0.965		
<u> </u>	77	total Wiener path no.	0.903	0.892		
<u> </u>	78	Shannon Index	0.911	0.911		
<u></u>		total no. of paths	0.939	0.932		
L		Bonchev-Trinajstić IdW index	0.958	0.955		
<u> </u>		Bonchev-Trinajstić mean IdW	•			. <i>.</i>
	81	index	0.972	0.972		
<u> </u>	82	Bonchev-Trinajstić IdC index	0.979	0.978		-
	` {	Bonchev-Trinajstić mean IdC			ţ	C C
1	83	index	0.793	0.773	0.757	0.739
	84	Wiener parity no.	0.988	686.0		
	85	Platt F no.	0.996	0.997		
	86.	Delta partition I	0.996	966:0		
	87	Delta partition 2	0.992	0.992		
	. 88	Delta partition 3	0.997	0.997		
	89	Delta partition 4	0.995	966.0		-
	90	Delta partition 5 <sup>1</sup>	1.000	1.000		
	ij	Delta partition 61	1.000	1.000		
	9.2	No. H	0.996	0.997		
	93	No. B <sup>1</sup> ·	1.000	1.000		
	94	No. C	0.997	0.998		
ĹJ	95	No. N	0.995	0.995		
	96	No. O	0.994	0.993		
	. <b>7</b> 6	No. F	966'0	966.0		
<u></u>	98	No. Si <sup>1</sup>	1.000	1.000		-
	66	No. P	0.999	0.999		

F16. 9D

		SISO	SISO	CSIM	MISO
		Training	Test	Training	Test
Index	Descriptor	$\mathbb{R}^2$	$\mathbb{R}^2$	$\mathbb{R}^2$	R <sup>z</sup>
100	No. S	. 0.997	0.999		
101	No. CI	0.997	0.997		
102	No. Ge <sup>1</sup>	1.000	1.000		
103	No. As <sup>1</sup>	1.000	1.000		
104	No. Se <sup>1</sup>	1.000	1.000		
105	No. Br	1.000	1.000		
106	No. I	1.000	1.000		
107	No. halogens	0.997	0.998		
108	Total topological state 1	0.924	0.918		:
109	Total topological state 2	0.947	0.945		
110	Total topological state 3	0.904	0.888		
111	Total topological state 4.	0.956	0.956		
112	Total topological state 5	0.852	0.826	0.915	0.907
113	Total topological state 6	0.980	0.980		
114	Total topological state 7	0.832	0.790	0.914	0.898
115	Total topological state 8	0.988	0.988		
116	Total topological state 9	0.913	0.909		•
117	Total topological state 10	0.922	0.918		

F16. 9E

Lead	Random	Direct	SISO/MISO	SISO/MISO	PC-MISO	PC-MISO
	Similarity	Similarity	Similarity	Identity	Similarity	Identity
1	1.754	0.480	0.501	%69	0.486	. 86%
. 2	1.158	0.238	0.279	26%	0.244	83%
3	1.664	0.655	0.680	64%	0.660	84%
4	1.291	0.179	0.213	%09	0.186	76%
. 5.	1.763	0.327	0.335	82%	0.334	83%
9	1.196	0.201	0.224	58%	0.209	75%
7	1.294	0.274	0.291.	72%	0.283	77%
∞	1.385	0.268	0.288	73%	0.275	84%
δ.	1.694	0.464	0.481	74%	0.470	86%
10	1.613	0,460	0.470	79%	0.464	87%
					¥	

F16. 10

16.

.3<sup>7</sup> .:

•

F16, 12

Tray

18 B

13

 $(-1)^{-\frac{1}{2}}$ 

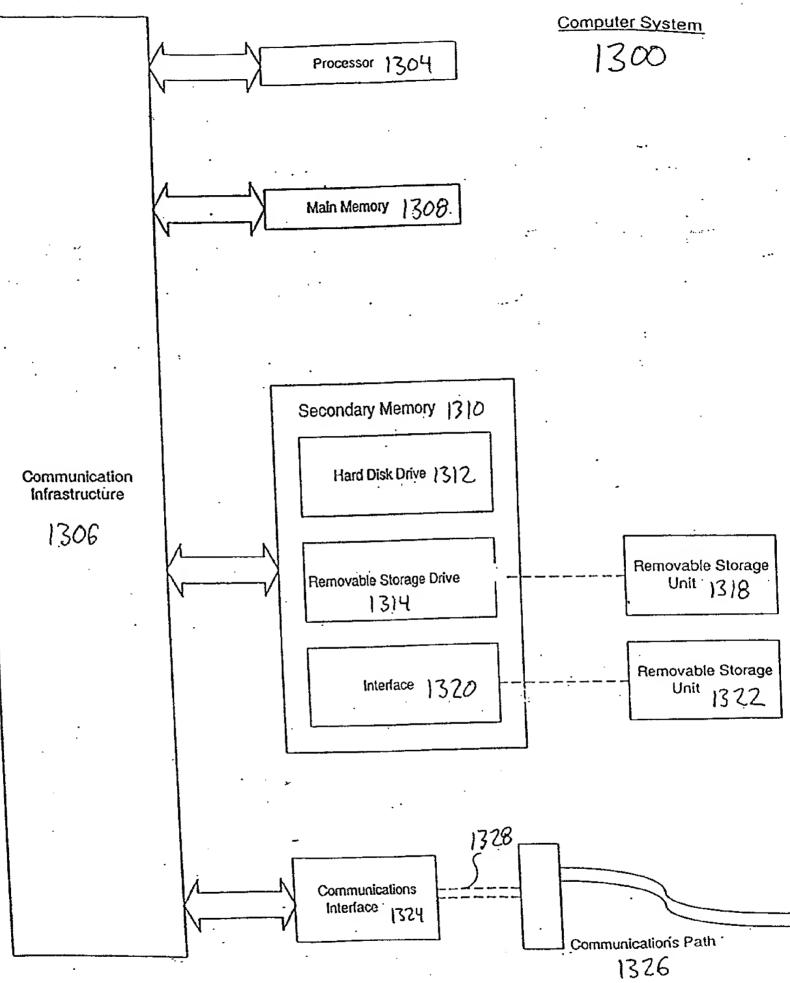


FIG.